Developments in numerical methods (I)

WGNE-meeting, DWD, Offenbach, Germany
24-27 Sept. 2019

Michael Baldauf (DWD)

1. report from the ‚PDEs on the sphere 2019'
2. Planned development at DWD

PDEs on the sphere

29 April – 03 May 2019, Montreal, Kanada

- first workshop 1990, takes place every ~18 months
- All aspects of dynamical core formulation
- Coupling between equations and with sub-grid scale parametrisations
- Parallel scaling
- Test cases
- Equation sets

PDEs
THE WORKSHOP ON PARTIAL DIFFERENTIAL EQUATIONS ON THE SPHERE

- Mostly presentations about meteorology
(+ 2* ocean modelling, 2* solar physics)
- presentations a 20 min. (+ several posters)
- about 70 participants (16 Can, 12 UK, 11 USA, 11 D, 6 F, …)
- http://collaboration.cmc.ec.gc.ca/science/pdes-2019/index-en.html

Most prominent topics this year

•**mixed/compatible finite elements**
(talks by Melvin, Lee, Wimmer, Shipton, Gibson, Bendall)
→ actual development at UK MO: GungHo/LFRic-project
cubed sphere, better separation between computational and science code;
users desired improved conservation properties

•**spectral elements** (=**continuous Galerkin**)
(talks by Reineke, Taylor, Lauritzen)

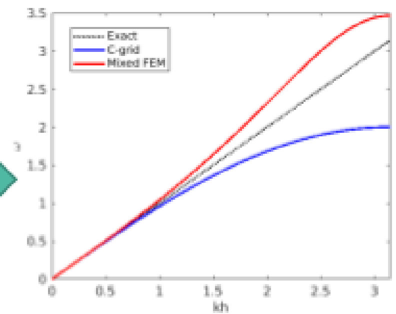
- US Navy: Operationalisation of NEPTUNE planned for ~2025
(NH, spectral element, cubed sph.)
- E3SM (Energy Exascale Earth System Model) used by 8 DOE labs + univ.
(HOMME-NH dyn core: horiz: SE, HEVI-IMEX)
→ mimetic horizontal differencing → mass & energy conservation

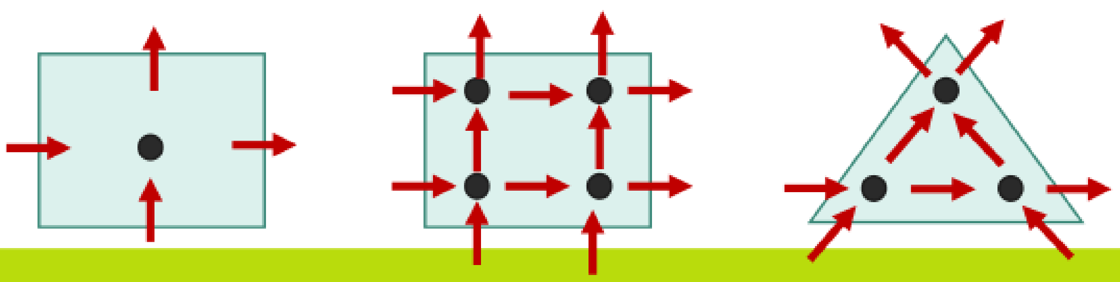
•time integration: **exponential integrators**
(talks by Côté, Peixoto, Gaudreault)
is a topic since years, but seems not yet used/planned for operational models

Mixed Finite Elements

Mixed Finite Element method gives

- Compatibility: $\nabla\times\nabla\varphi = 0, \nabla\cdot\nabla\times\boldsymbol{v} = 0$
- Accurate balance and adjustment properties
- No orthogonality constraints on the mesh
- Flexibility of choice mesh (quads,triangles) and accuracy (polynomial order)





Thomas Melvin (UK MO)

Motivation 2 - Exponential integration with nonlinear advection

- Exponential integrators solve accurately **linear** problems
  - Usually allows very large timesteps

$$\frac{dU}{dt} = LU, \quad U(0) = U_0,$$

$$U(t_{n+1}) = e^{\Delta t L} U(t_n),$$

- For nonlinear equations
  - Usually nonlinearity limits timestep sizes

$$\frac{dU}{dt} = LU + N(U), \quad U(0) = U_0,$$

$$U(t_{n+1}) = e^{\Delta t L} U(t_n) + e^{\Delta t L} \int_{t_n}^{t_{n+1}} e^{-(s-t_n)L} N(U(s)) ds,$$

Goal2

How to treat N if dominated by nonlinear advection, in way to allow large time step sizes?

Some other statements:

- P. Lauritzen: total energy budgets
  - „Conserving total energy to within ~0.01 W/m² is considered ‚good enough' for coupled climate modeling"
    compare: the earths energy imbalance is ~ 1 W/m²
  - In CAM-SE: total energy errors in the dyn. core, physics-dynamics coupling and pressure work errors are ~-0.6 … +0.3 W/m².
    Local erros can be an order of magnitude larger (at least).
- Xi Chen:
  grid-staggering becomes increasingly less important for higher-order methods

A possible alternative dynamical core for ICON based on Discontinuous Galerkin Discretisation

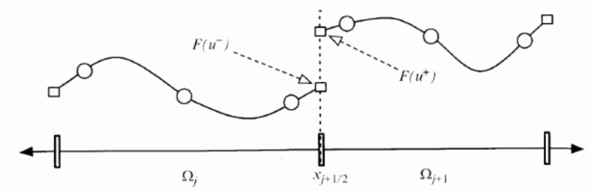
Michael Baldauf (Deutscher Wetterdienst)

MetStröm

ESCAPE

Discontinuous Galerkin (DG) methods in a nutshell

$$\frac{\partial q^{(k)}}{\partial t} + \nabla \cdot \mathbf{f}^{(k)}(q) = S^{(k)}(q), \qquad k = 1, ..., K$$



From *Nair et al. (2011)* in *‚Numerical techniques for global atm. models'*

weak formulation $\int_{\Omega_j} dx \, v(\mathbf{x}) \cdot \ldots$

Finite-element ingredient

$$q^{(k)}(x,t) = \sum_{l=0}^{p} q_{j,l}^{(k)}(t) \; p_l(x - x_j)$$

e.g. Legendre-Polynomials

e.g.
Cockburn, Shu (1989) Math. Comput.
Cockburn et al. (1989) JCP
Hesthaven, Warburton (2008): Nodal DG Methods

Finite-volume ingredient

$$\mathbf{f}(q) \rightarrow \mathbf{f}^{num}(q^+, q^-) = \frac{1}{2}\left(\mathbf{f}(q^+) + \mathbf{f}(q^-) - \alpha(q^+ - q^-)\right)$$

Lax-Friedrichs flux

Gaussian quadrature for the integrals of the weak formulation

→ ODE-system for $q^{(k)}{}_{jl}$

DG – Pros and Cons

Deutscher Wetterdienst
Wetter und Klima aus einer Hand

- **local conservation**
- any **order of convergence** possible
- flexible application on **unstructured grids** (also dynamic adaptation is possible, h-/p-adaptivity)
- very good **scalability**
- **explicit** schemes are easy to build and are quite well understood
- higher accuracy helps to **avoid several awkward approaches** of standard 2nd order schemes: staggered grids (on triangles/hexagons, vertically heavily stretched), numerical hydrostatic balancing, grid imprints by pentagon points or along cubed sphere lines, …

- high computational costs due to
  - (apparently) **small Courant numbers**
  - higher number of DOFs
- **well-balancing** (hydrostatic, perhaps also geostrophic?) in Euler equations is an issue (can be solved!)
- basically ‚only' an **A-grid-method**, however, the ‚spurious pressure mode' is very selectively damped!

Target system: **ICON model**
(Zängl et al. (2015) QJRMS)

- operational at DWD since Jan. 2015
  (global (13km) and nest over Europe (6.5km))
- convection-permitting (2.2km): Q4/2020
- horiz.: icosahedral triangle C-grid, vertic.: Lorenz-grid
- non-hydrostatic, compressible
- mixed finite-volume / finite-difference (mass, tracer mass conservation)
- predictor-corrector time-integration → overall 2nd order discretization

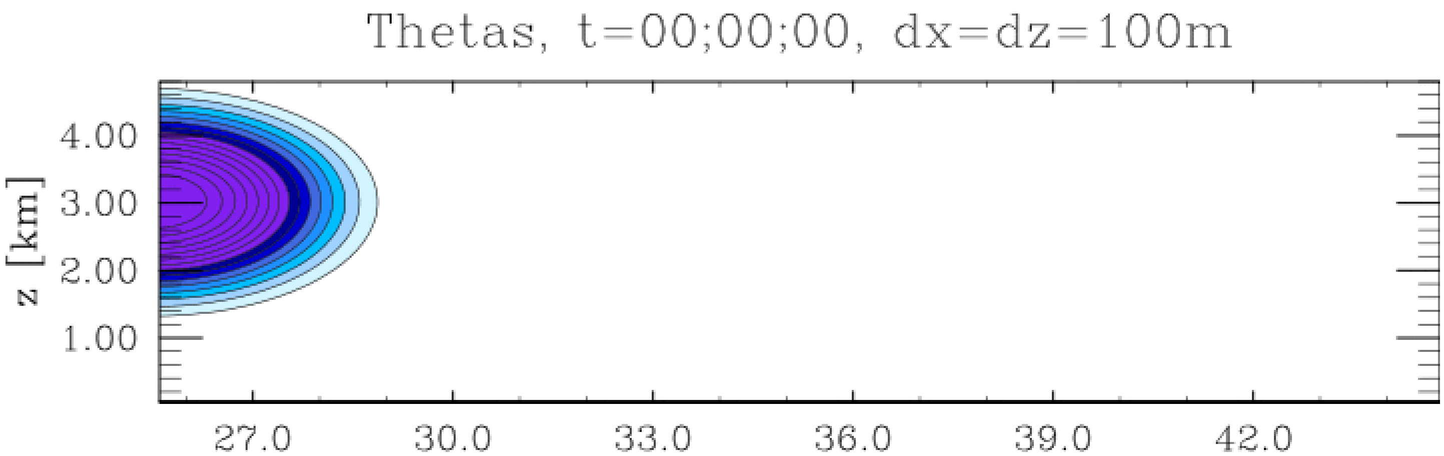
---

but currently far away from this, only a **toy model for 2D problems exists** with:

- explicit time integration DG-RK (with Runge-Kutta schemes) or
  horizontally explicit-vertically implicit (DG-HEVI) (with IMEX-Runge-Kutta)
- ‚local DG' (LDG) option for PDEs with higher spatial derivatives
- use of a triangle grid (also on the sphere) is optional

Test case: falling cold bubble

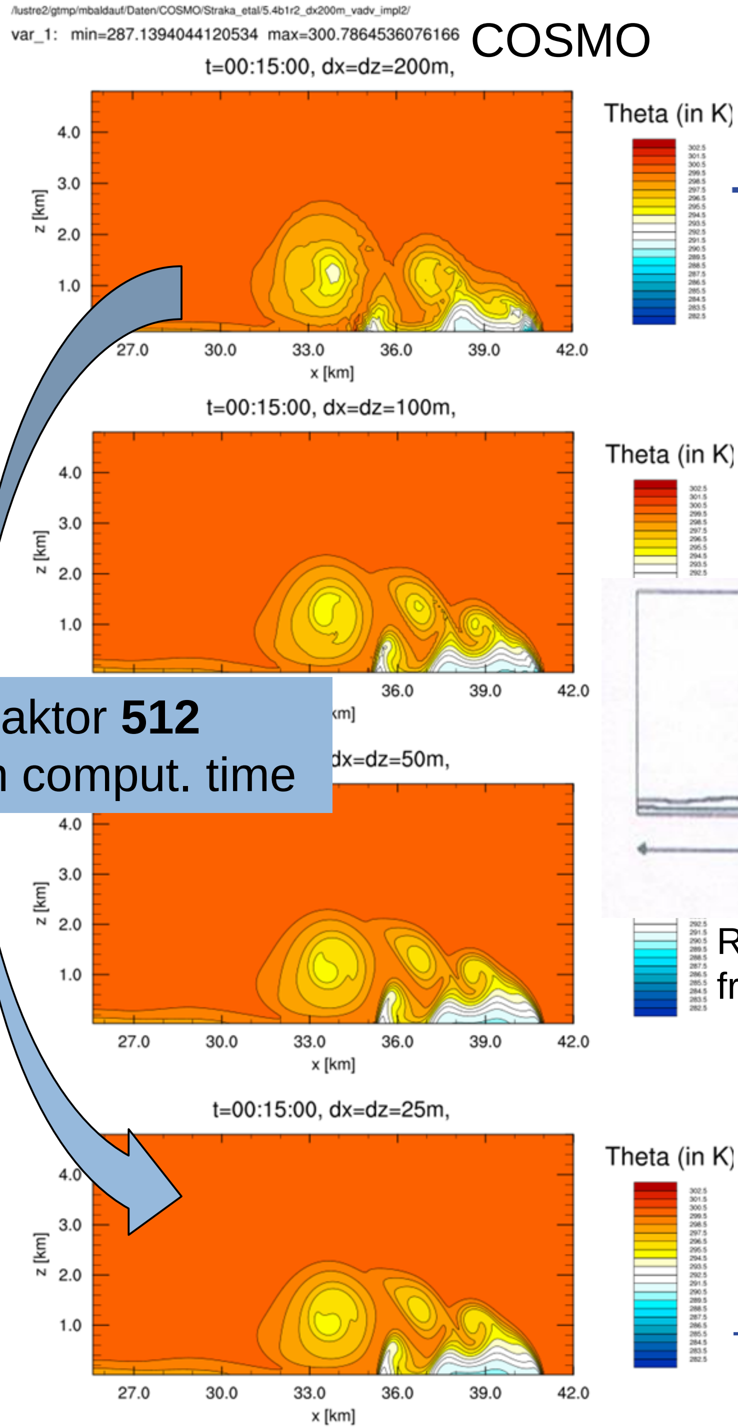
Testsetup by *Straka et al (1993)*



Test properties:

- test of dry Euler equations (without Coriolis force)
- unstationary
- strongly nonlinear
- comparison with reference solution from paper

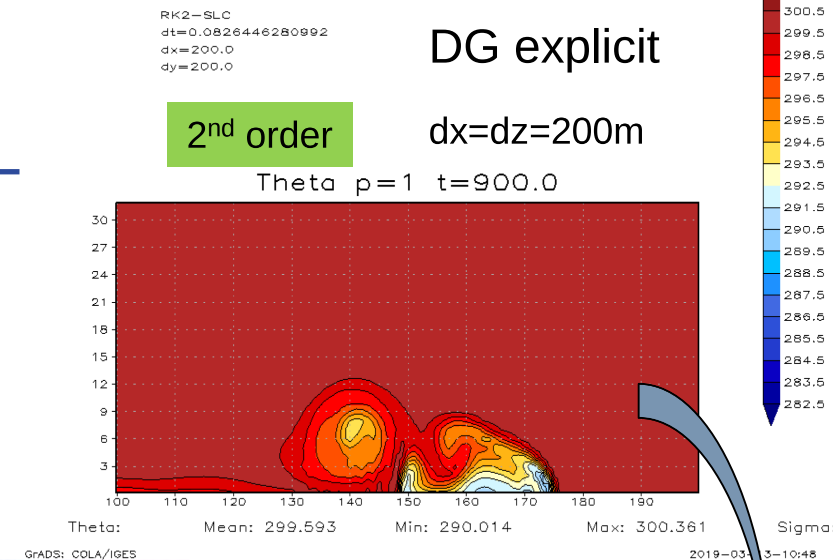
COSMO



Faktor **512** in comput. time

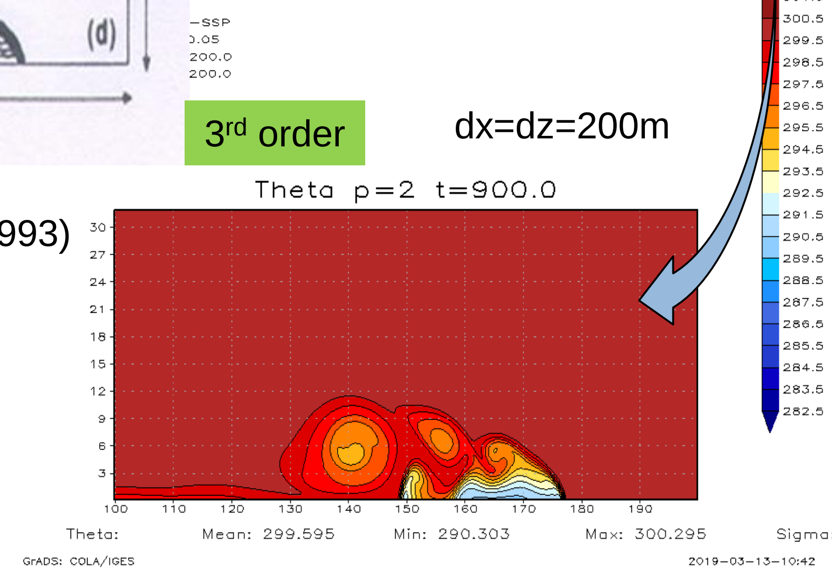
DG explicit

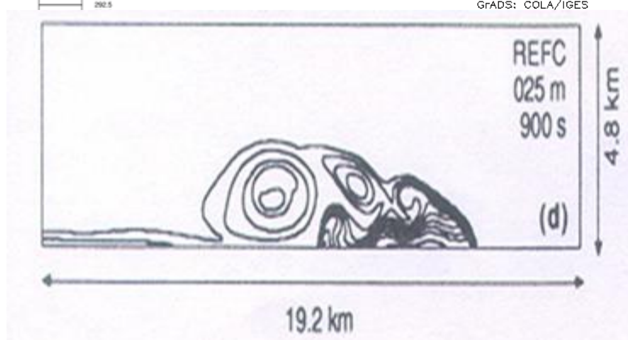
2nd order dx=dz=200m



Faktor **4.3** in comput. time

3rd order dx=dz=200m





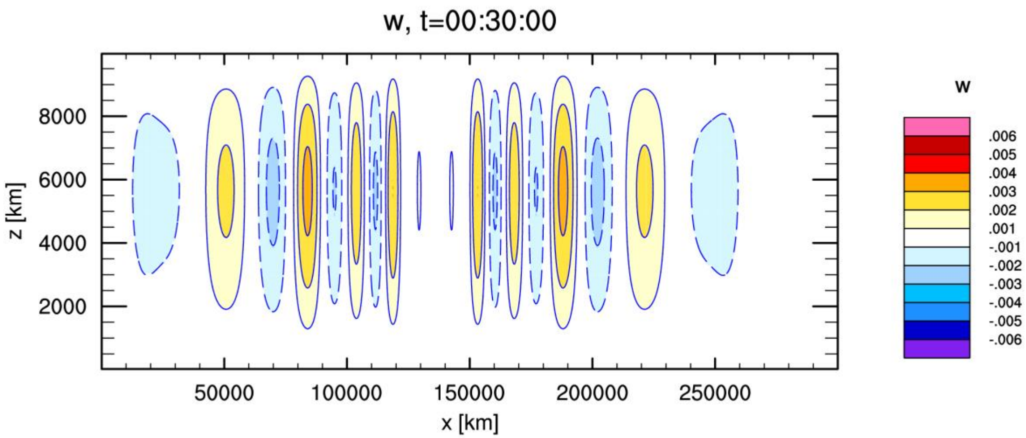
Reference solution from Straka et al. (1993)

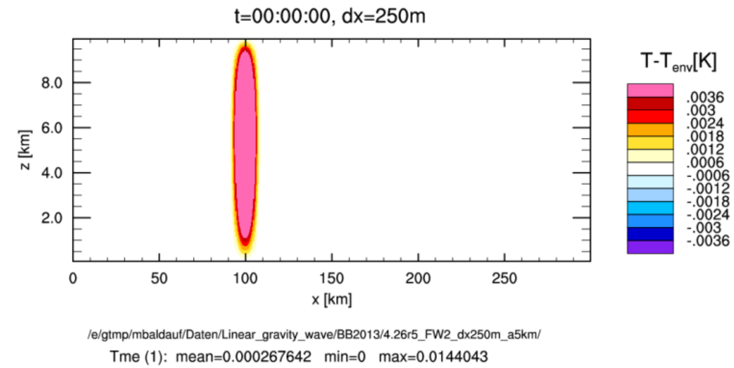
Linear gravity/sound wave expansion in a channel

Deutscher Wetterdienst
Wetter und Klima aus einer Hand

setup similar to *Skamarock, Klemp (1994) MWR*

Δx=500m, Δz=250m

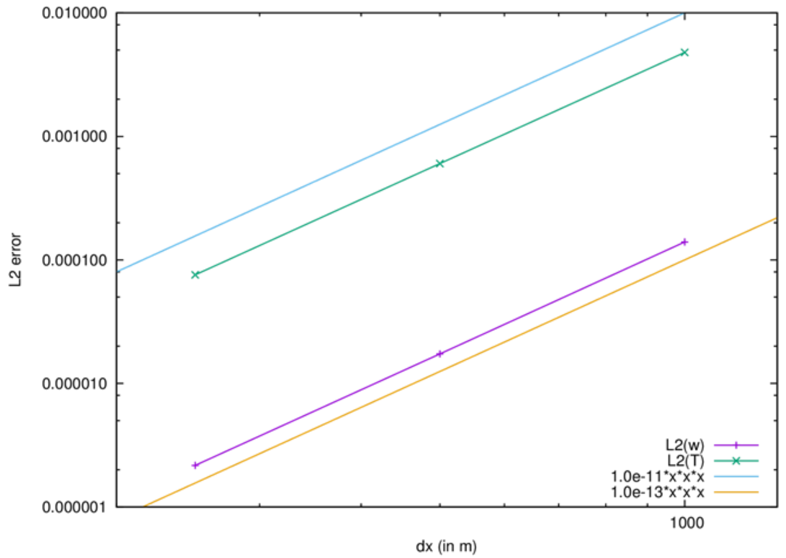




colors : simulation with p=2/RK3-SSP
(i.e. 3[rd] order explicit DG)

blue lines: analytic solution for compressible, non-hydrostatic Euler eqns.
(*Baldauf, Brdar (2013) QJRMS*)

Exact 3[rd] order convergence for w and T‘:



Horizontally explicit - vertically implicit (HEVI)-scheme with DG

Motivation: get rid of the strong time step restriction by vertical sound wave expansion in flat grid cells (in particular near the ground)

$$\frac{\partial q^{(s)}}{\partial t} + \underbrace{\nabla \cdot \mathbf{f}^{(s)}_{slow}}_{\text{explicit}} + \underbrace{\nabla \cdot \mathbf{f}^{(s)}_{fast}}_{\text{implicit}} = \underbrace{S^{(s)}_{slow}}_{\text{explicit}} + \underbrace{S^{(s)}_{fast}}_{\text{implicit}}$$

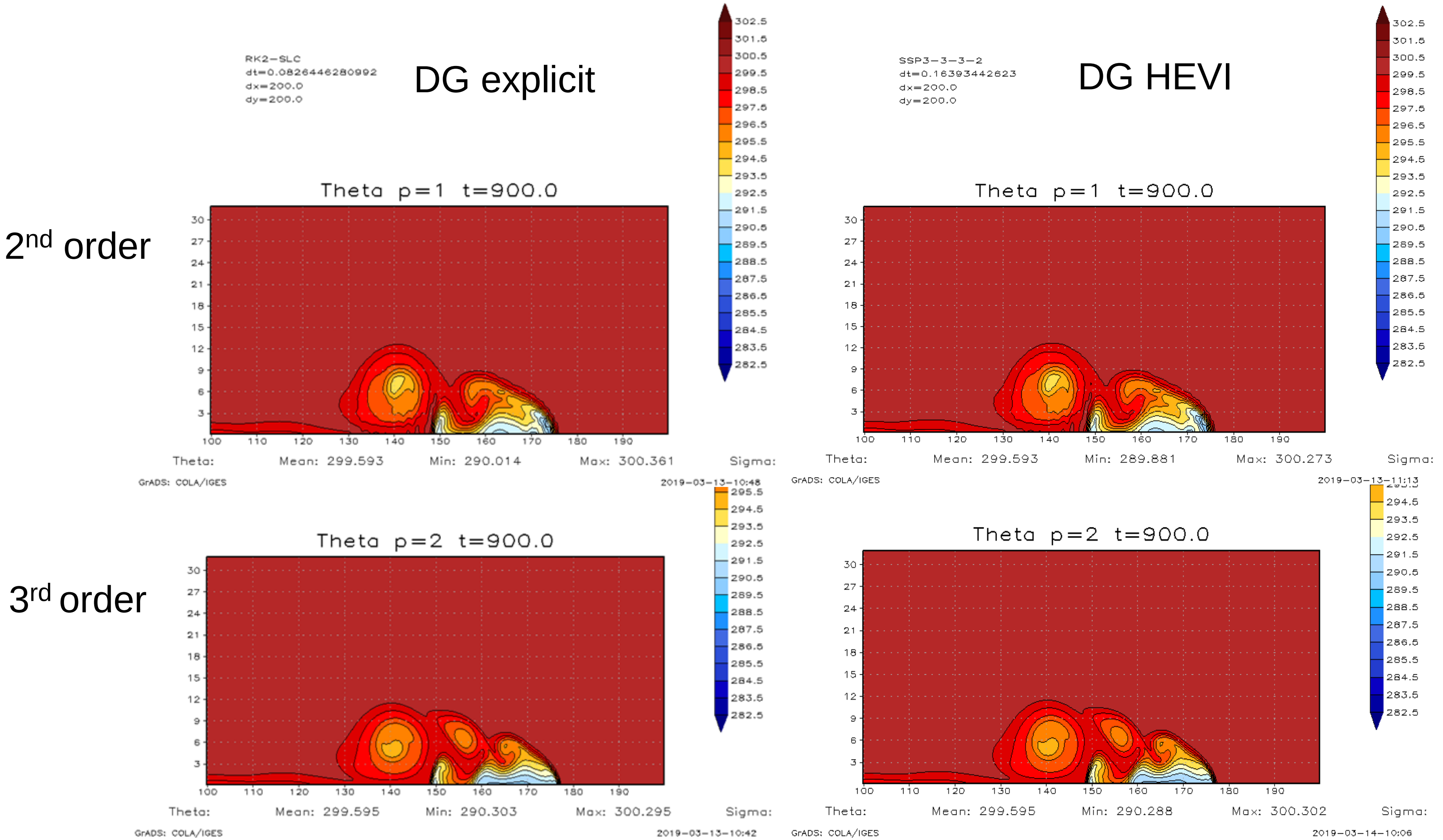
$$\mathbf{f}^{(s)}_{fast} = f^{(s)}_{z,fast}\mathbf{e}_z$$

$$f^{(s)}_{z,fast} = \sum_{s'} H^{ss'} q^{(s')}$$

- Use of IMEX-RK (SDIRK) schemes: SSP3(3,3,2), SSP3(4,3,3) (*Pareschi, Russo (2005) JSC*)
- The implicit part leads to several band diagonal matrices
  → here a direct solver is used (expensive!)

References:
Giraldo et al. (2010) SIAM JSC: propose a HEVI semi-implicit scheme
Bao, Klöfkorn, Nair (2015) MWR: use of an iterative solver for HEVI-DG
Blaise et al. (2016) IJNMF: use of IMEX-RK schemes in HEVI-DG
Abdi et al. (2017) arXiv: use of multi-step or multi-stage IMEX for HEVI-DG

Test case: falling cold bubble (Straka et al. (1993)
Comparison explicit vs. HEVI scheme



How to bring DG on the sphere …

Idea to avoid pole problem and to keep high order discretization:
use **local (rotated) coordinates** for every (triangle) grid cell,
i.e. rotate every grid cell towards λ≈0, φ≈0.
→ geometry is treated exactly
→ transform fluxes between neighbouring cells

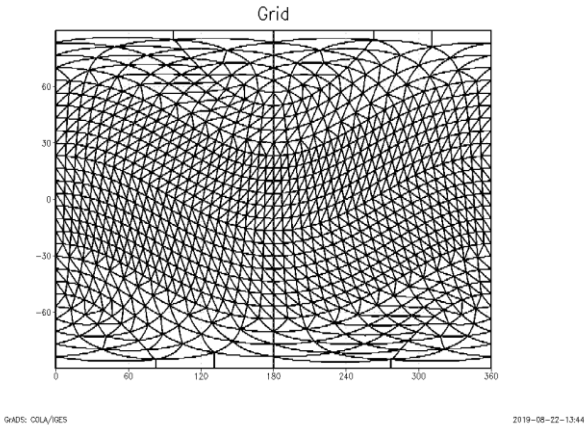
shallow water equations
covariant formulation (here: without bathymetry)

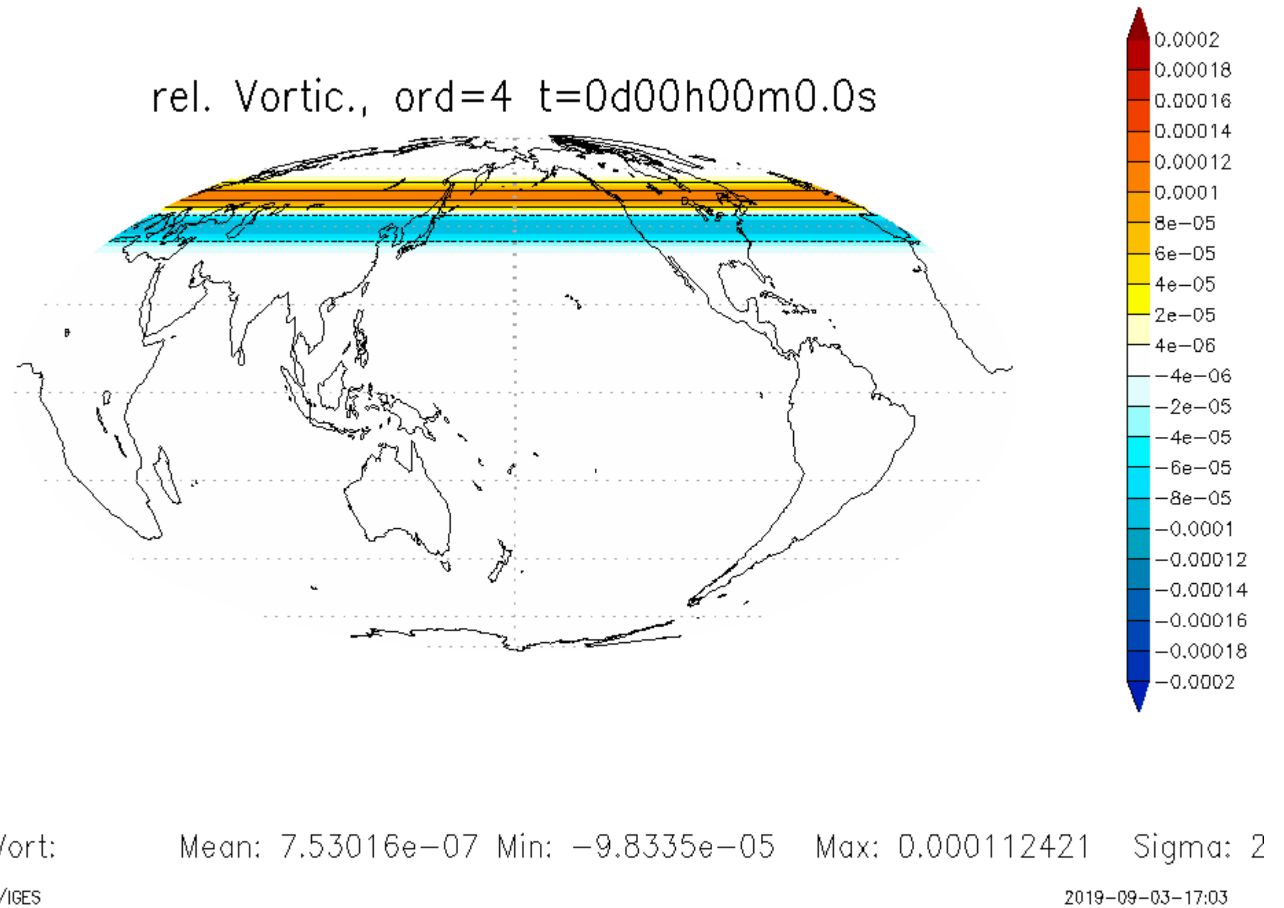
$$\begin{aligned}
\frac{\partial \sqrt{G} H}{\partial t} + \frac{\partial}{\partial x^i} \sqrt{G} m^i &= 0 \\
\frac{\partial \sqrt{G} m^i}{\partial t} + \frac{\partial}{\partial x^j} \sqrt{G} T^{ij} &= \sqrt{G}\left(F^i_{Cor} - \Gamma^i_{jk} T^{jk}\right) \\
T^{ij} &= \frac{m^i m^j}{H} + \frac{1}{2} g^{ij} g_{grav} H^2
\end{aligned}$$

Barotropic instability test
Galewsky et al. (2004)

4th order DG scheme
without additional diffusion
dx~67 km, dt=15 sec.

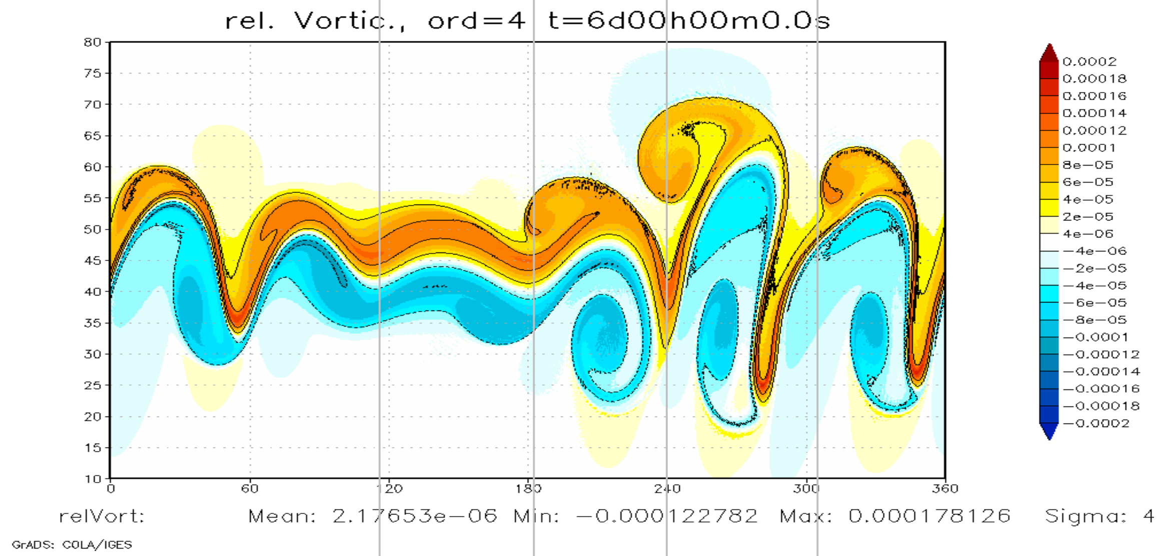
simple triangle grid
on the sphere
dx ~ 500km:





Barotropic instability test
Galewsky et al. (2004)

relative vorticity



4th order DG scheme
without additional diffusion
dx~67 km, dt=15 sec.

FMS-SWM (Geophys. Fl. Dyn. Lab.)
without additional diffusion
dx~60 km (T341), dt=30 sec.

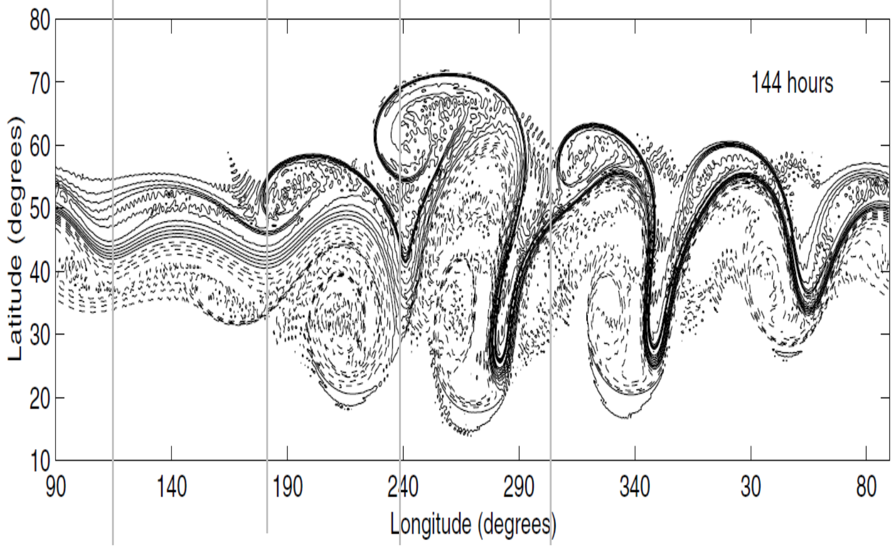


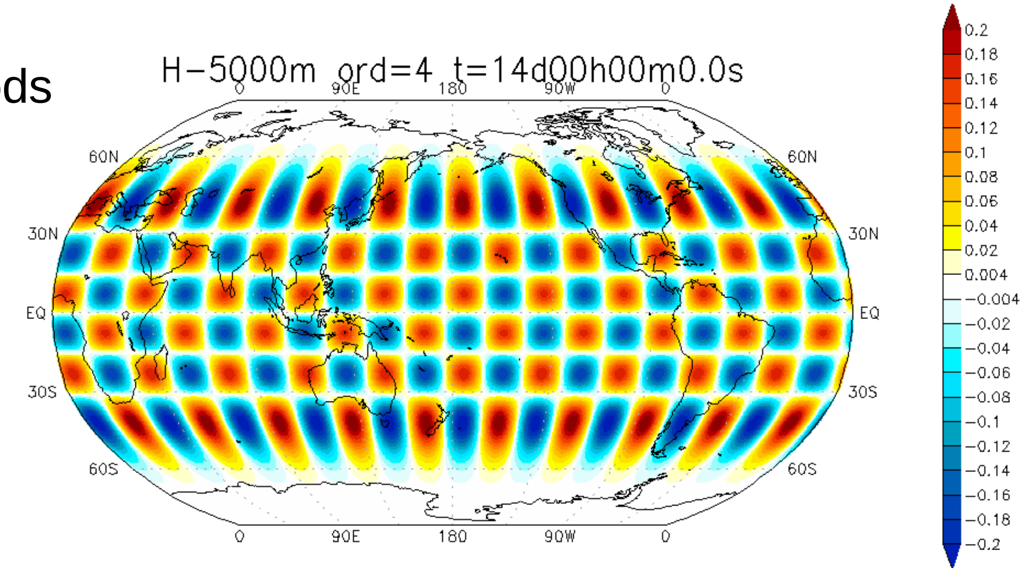
Fig. 4 from *Galewsky et al. (2004)*

Linear inertial-gravity wave

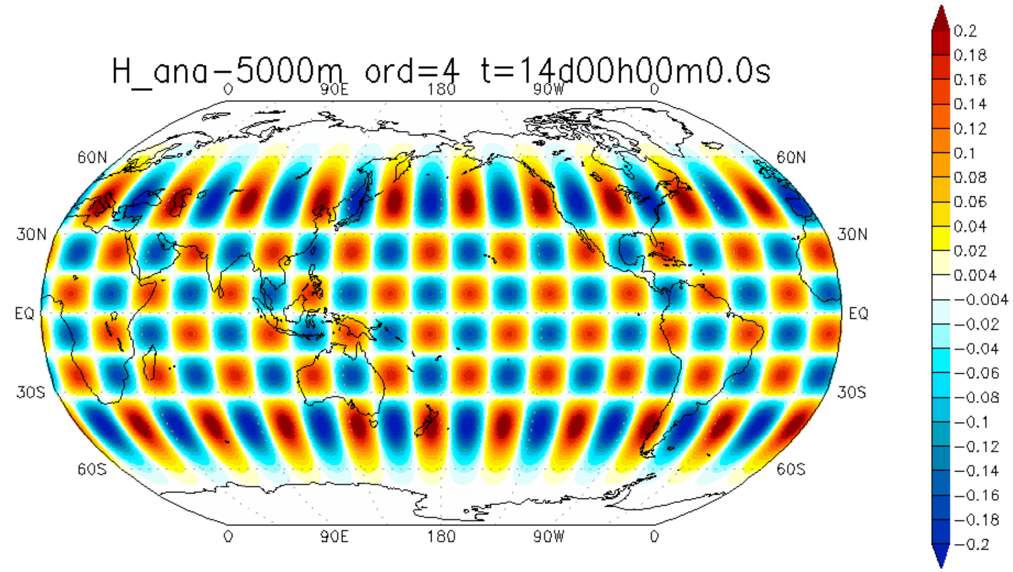
Solution after 14 days ~ 100 periods

4th order DG scheme
without additional diffusion
dx~134 km, dt=30 sec.

→ wave pattern remains stable



Analytic solution by
Shamir, Paldor (2016),
Paldor (2013)
(is known to be slightly too fast
by ~0.3% ~0.3 wavelengths)
This test case might possibly replace the well-known 'Rossby-Haurwitz wave test' in the future.



Summary

- **2D toy model** for
  - explicit DG-RK (on arbitrary unstructured grids with triangle or quadrilateral grid cells) and
  - **HEVI DG-IMEX-RK**

  works for several idealized tests (also Euler equations with terrain-following coordinates), correct convergence behaviour, …
- **DG on the sphere** by use of local (rotated gnomonial) coordinates

Outlook

- **further design decisions**: nodal vs. modal, local DG vs. interior penalty vs. …, …
- coupling of **tracer advection** (mass-consistency)?
- improve **efficiency** in the HEVI direct solver
- further **milestones** (for the next years!)
  - development of a 3D prototype DG-HEVI solver
  - choose optimal convergence order *p* and grid spacing
    estimated: $p_{horiz} \sim 3 \ldots 6$, $p_{vert} \sim 3 \ldots 4$ ($p_{time} \sim 3 \ldots 4$)

PDEs
The Workshop on Partial Differential Equations on the Sphere

Announcement:

The next

„Partial differential equations on the sphere“ – workshop

will take place at
DWD, Offenbach, Germany
5-9 October 2020